AMENDMENT TRANSMITTAL LETTER (Large Entity) Applicant(s): **Schuppert et al.**					Docket No. **100717-574US**
Application No. **10/511,231**	Filing Date **10/12/04**	Examiner **Adrian L. Kennedy**	Customer No. **23526**	Group Art Unit 2121	Confirmation No. **9226**

Invention: **Method and Computer for Experimental Design**

COMMISSIONER FOR PATENTS:

Transmitted herewith is an amendment in the above-identified application.

The fee has been calculated and is transmitted as shown below.

CLAIMS AS AMENDED

	CLAIMS REMAINING AFTER AMENDMENT		HIGHEST # PREV. PAID FOR		NUMBER EXTRA CLAIMS PRESENT		RATE	ADDITIONAL FEE
TOTAL CLAIMS	23	-	22	=	1	x	$50.00	$50.00
INDEP. CLAIMS	2	-	3	=	0	x	$200.00	$0.00
Multiple Dependent Claims (check if applicable) ☐								$0.00
TOTAL ADDITIONAL FEE FOR THIS AMENDMENT								$50.00

☐ No additional fee is required for amendment.

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IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

In re Patent Application of:

SCHUPPERT *et al.*

Serial No. 10/511,231

Filed: October 12, 2004

For: METHOD AND COMPUTER
FOR EXPERIMENTAL DESIGN

Examiner: Kennedy, Adrian L.

Group Art Unit: 2121

March 26, 2007

Commissioner for Patents
Alexandria, VA 22313-1450

Amendment and Response under 37 C.F.R. § 1.111

Sir:

In response to the Official Action dated October 3, 2006, please amend the above-identified application as follows. A request for a three (3) month extension of time accompanies this response.

Amendments to the Specification are reflected in the paragraphs reproduced beginning on page 2 of this paper.

Amendments to the Claims are reflected in the listing of claims beginning on page 4 of this paper.

Remarks/Arguments begin on page 9 of this paper.

Amendments to the Specification

Please amend paragraph [0016] of the substitute specification as follows:

[0016] In a preferred embodiment, a computer based system for designing experiments includes a meta layer module which uses a priori and supplementarily obtained knowledge to influence processing operations at an optimizer, thereby effectively tuning the optimizer. The knowledge preferably includes rules associated with interactions, such as rules relating to structure-interaction with data mining and other methods. The rules can be integrated in the processing the optimizer performs for designing experiments at to influence the optimizer processing before, during or after an optimization processing step, or even continuously.

Between paragraphs [0017] and [0018] of the substitute specification, please insert the following:

In a preferred embodiment, the inventive method for designing experiments for achieving an optimization goal has the following steps: A) selection of at least a first experiment from an experimental space by means of a data-driven optimizer in a computer unit; B) inputting of experimentally determined experiment data of the first experiment in at least one meta layer into a computer unit; C) use of at least one meta layer for the evaluation of the experiment data; D) inputting of the experimentally determined experiment data of the first experiment into the data driven optimizer; E) influencing of the data driven optimizer by the result of the evaluation in the meta layer and checking the goal achieved; F) selection of at least a second experiment from the experimental space by means of the data-driven optimizer; G) repetition of steps B) to E) for the data of the second experiment; and H) stopping the method on achieving the goal or repeating steps A) to F) for at least a third or subsequent experiments until the

goal has been achieved.

The method is repeated until the optimization goal has been achieved or until it is concluded that it may not be possible to achieve the optimization goal. The method can be terminated automatically or by the user. The optimization goal may be to reach certain evaluation characteristic numbers for the experiments. The characteristic numbers may, for example, be yield selectivities, space time yields, costs, physical properties, action mechanisms, derived properties, etc. It is also possible to evaluate the experiments using a plurality of characteristic numbers.

Please amend paragraph [0045] of the substitute specification as follows:

[0045] The module 13, if appropriate, re-evaluates an experiment or experiments, based on the rules and secondary conditions contained in the module 12. In a preferred embodiment, an experiment is re-evaluated only if a predefined threshold value is exceeded. Alternatively, the user can intervene to activate or deactivate the re-evaluation. The re-evaluation may include assigning a worse evaluation to experiments recognized as being poor and an improved evaluation to experiments recognized as being good. The optimizer 6 processes the data supplied from the module 9, which includes the data file from ~~in~~ the module 8, and ~~which~~, if appropriate, ~~contains~~ re-evaluated experiment data, to create a further experiment design which is then representatively stored as data in the experiment design module 14. The experiment set-up module 7 then performs experiments corresponding to the experiment designs stored in the module 14.

AMENDMENTS TO CLAIMS

Claims 1-21 (canceled)

22. (currently amended) A method for designing experiments comprising the steps of:

a) selecting at least a first experiment from an experimental space including a plurality of experiments using a data-driven optimizer;

b) ~~receiving~~ inputting experimentally determined experiment data of the first experiment to at least one meta layer module;

c) evaluating the experimentally determined experiment data of the first experiment at a the meta layer module, wherein the meta layer module generates evaluation data based on the evaluating of the experimentally determined experiment data; ~~and~~

d) processing the experimentally determined experiment data of the first experiment at the optimizer, wherein the processing at the optimizer is influenced by the evaluation data and wherein the optimizer generates experiment design data based on the processing of the experimentally determined experiment data; and

e) outputting an experiment design based on the experiment design data.

23. (currently amended) The method of claim 22 further comprising the ~~step~~ steps of:

f) inputting an optimization goal;

g) selecting at least a second experiment from the experimental space using the optimizer;

h) performing step b) to step d) for experimentally determined experiment data of the second experiment; and

i) continuing to perform steps g) and h) until the optimization goal is reached.

24. (currently amended) The method of claim 23 ~~22~~, wherein at least one of the optimizer and the meta layer module changes the experimental space before the selecting the at least ~~one~~ second experiment step.

25. (previously presented) The method of claim 22, wherein the meta layer module contains at least one of a neural network module, a hybrid model module, a rigorous model module and a data mining module.

26. (currently amended) The method of claim 22, wherein the ~~experimental~~ experiment data is based on experiments from at least one of active ingredient research, materials research, catalysis research, biotechnology and optimization of reaction conditions.

27. (previously presented) The method of claim 22, wherein the evaluating at the meta layer module to generate the evaluation data includes the step of filtering the experiment data.

28. (previously presented) The method of claim 27, wherein the filtering includes re-evaluating the experiment data.

29. (previously presented) The method of claim 27, wherein the filtering includes at least one of weighting and pre-selecting the experiment data.

30. (previously presented) The method of claim 29, wherein the weighting includes at least one of using a weighting parameter and performing at least one duplication of the experiment data.

31. (previously presented) The method of claim 22, wherein the optimizer includes at least one core module and one module for selecting new test points.

32. (currently amended) The method of a claim 31, wherein the processing at the optimizer is influenced based on processing at the module for selecting the new test points.

33. (currently amended) The method of a claim 32, wherein the processing at the module for selecting the new test points is influenced by at least one of a value exceeding a threshold and a predefined user value.

34. (previously presented) The method of claim 31, wherein the processing at the optimizer is influenced based on processing at the core module.

35. (previously presented) The method of claim 34, wherein processing at the core module is influenced by at least one of a value exceeding a threshold and a predefined user value.

36. (currently amended) A system for designing experiments comprising:

an experimental space module including a plurality of experiments;

an experiment data module including experimentally determined experiment data for at least one of the experiments in the experimental space module;

a optimizer for selecting at least one first experiment from ~~an~~ the experimental space module; ~~and~~

a meta layer module coupled to the optimizer for receiving experimentally determined experiment data of the first experiment from the experiment data module;

wherein the meta layer module evaluates the experimentally determined experiment data and generates evaluation data based on the evaluation of the experimentally determined experiment data;

wherein the optimizer processes the experimentally determined experiment data of the first experiment and generates experiment design data based on the processing of the experimentally determined experiment data of the first experiment, wherein the processing by the optimizer is influenced by the evaluation data; and

wherein the optimizer outputs to the experimental space module an experiment design based on the experiment design data ~~evaluating experiment data determined experimentally for the first experiment, wherein the meta layer module generates experiment design data for influencing processing at the optimizer~~.

37. (previously presented) The system of claim 36, wherein the meta layer module includes at least one of a neural network module, a hybrid model module, a rigorous model module and a data mining module.

38. (previously presented) The system of claim 36, where the meta layer module includes a filtering module for filtering the experiment data.

39. (previously presented) The system of claim 38, wherein the filtering module is operable to re-evaluate the experiment data.

40. (previously presented) The system of claim 38, wherein the filtering module is operable to perform at least one of weighting and pre-selecting the experiment data.

41. (previously presented) The system of claim 36, wherein the optimizer includes at least one core module and a module for selecting new test points.

42. (currently amended) The system of a claim 41, wherein the meta layer module is operable to influence the module for selecting the new test points.

43. (currently amended) The system of ~~according~~ claim 41, wherein the meta layer module is operable to influence the core module.

44. (new) The system of claim 36, wherein the system is for achieving an optimization goal, and wherein, until the optimization goal is reached as determined by the optimizer or the meta layer module,

(a) the optimizer selects at least one second experiment from the experimental space module;

(b) the meta layer module receives experimentally determined experiment data of the second experiment from the experiment data module, evaluates the experimentally determined experiment data of the second experiment and generates evaluation data based on the evaluation of the experimentally determined experiment data of the second experiment; and

(c) the optimizer processes the experimentally determined experiment data of the second experiment and generates experiment design data based on the processing of the experimentally determined experiment data of the second experiment, wherein the processing by the optimizer is influenced by the evaluation data generated from the experimentally determined experiment data of the first and second experiments.

REMARKS

Claims 22-24, 26, 32-33, 36 and 42-43 have been amended, and claim 44 has been added. Claims 22-44 are presently pending.

The specification has been amended to clarify the description and to correct typographical errors uncovered during further review of the application. In addition, the specification has been amended to re-introduce the text at page 4, line 12-page 5, line 7 of the English language translation of International PCT/EP03/03424, which was filed with the request for entry into the national stage transmittal documents on October 12, 2004. The subject text portion inadvertently was deleted from the application by the Second Preliminary Amendment filed February 8, 2005. No new matter has been added based on the amendments to the specification.

In view of such amendments and the following remarks, reconsideration and allowance of the claims, as presently presented, are respectfully requested.

EXAMINER'S ACTION

The 35 U.S.C. § 101 Rejections

Claims 22-43 were rejected under 35 U.S.C. § 101 ("Section 101") as being directed to non-statutory subject matter, because the claims do not set forth a "useful, concrete and tangible result." Independent method claim 22 and independent system claim 36, which have been amended to clarify what is the claimed invention, produce a practical, real world result, namely, an optimized experiment design.

Referring to amended claim 22, the claimed method for designing experiments sets forth a "useful" result, because the "experiment design" that is produced can be used, for example, in chemical research or a manufacturing process. (See specification, for example, at paragraphs [0007]-[0009]). For example, the experiment design may

include catalysts, active ingredients, materials or reaction conditions having "certain characteristic numbers" for a selected property, for example, yield selectivity, where the characteristic number of the selected property can impact a manufacturing process or a chemical reaction. (See specification, for example, at paragraphs [0007], [0010] and [0041], and the text portion introduced between paragraphs [0017] and [0018]).

In addition, the method of claim 22 generates a "concrete" result. In the claimed method, a meta layer module "generates evaluation data" based on experimentally determined experiment data. The "evaluation data" influences processing of the experimentally determined experiment data at an optimizer, where the optimizer generates the experiment design data from which an optimized experiment design is obtained. In the claimed method, each of the evaluation data, the experiment design data and the experiment design is determined based upon specific data and, furthermore, constitutes reproducible data.

Further, the method of claim 22 outputs the "experiment design", such that the experiment design is fixed and reportable data useful in a real world, practical application. For example, the outputted experiment design can be implemented as a method for controlling a manufacturing process or developing catalysts for a catalyzed reaction process. (See specification, for example, at paragraphs [0008], [0009] and [0041]).

As to claim 36, this claim is directed to a system for designing experiments that outputs "an experiment design" based on experiment design data generated at an optimizer. Claim 36 includes limitations corresponding to the limitations of claim 22 discussed above, such that claim 36, like claim 22, produces an experiment design having practical, real world applications.

Accordingly, claims 22 and 36, claims 23-35 and 37-43 which depend therefrom, and new claim 44 which depends from claim 36, are directed to statutory subject matter, and therefore, it is respectfully submitted that the rejections based on Section 101 should be withdrawn.

The 35 U.S.C. § 102 Rejections

Claims 22-43 were rejected under 35 U.S.C. § 102(b) as being anticipated by U.S. Patent No. 6,996,550 ("Wang *et al.*").

Independent claims 22 and 36, as amended, claims 23-35 and 37-43 which depend directly or indirectly upon claims 1 or 36, and new claim 44 depending from claim 36 clearly are patentable over Wang *et al.*

As discussed above, amended claim 22 is directed to a method for designing experiments where, in relevant part, a meta layer module generates evaluation data based on the meta layer module's evaluating experimentally determined experiment data of a first experiment. Further, claim 22 requires that the evaluation data influences processing of the experimentally determined experiment data of the first experiment at a data-driven optimizer. The influencing (tuning) of the optimizer using the evaluation data, which the meta layer module generates based on prior knowledge, *e.g.*, the experimentally determined experiment data, advantageously provides that the optimizer can rapidly converge upon an optimized experiment design, thereby reducing time and material expenditures. (See specification, for example, at paragraphs [0038], [0039] and [0041]).

In contrast to the claimed invention, although Wang *et al.* performs an optimization using configurations defined from a set of parameters (*e.g.*, materials having desired properties) and a set of constraints on physical operations of an

experimental device (see Wang *et al.* at Col. 4, ln. 46-56 and Col. 26, ln. 1-60), the Wang *et al.* optimization does not account for knowledge acquired from prior experimentation. Nowhere does Wang *et al.* teach or suggest generating evaluation data at a meta layer module, based on the meta layer module's evaluation of experimentally determined experiment data, in other words, prior experimentation knowledge, and then using the evaluation data to influence (tune) optimization processing of the experimentally determined experiment data at the optimizer, as required by claim 22.

Accordingly, claim 22 is patentable over Wang *et al.*

In addition, amended independent claim 36, which claims a system for designing experiments having limitations corresponding to those of claim 22 discussed above, is patentable over Wang *et al.* for the same reasons as set forth above with respect to claim 22.

Further, claims 23-35 and 37-44, which depend directly or indirectly upon claims 22 or 36, are also patentable over Wang *et al.* for the same reasons as set forth above with respect to claim 22 and because of the further restrictions they add.

Claims 23 and 44 require, in relevant part, iteratively processing experimentally determined experiment data of a plurality of experiments at the meta layer module and the optimizer, in the same manner as (set forth in claims 22 and 36, respectively,) for the experimentally determined experiment data for the first experiment, until an optimization goal is reached. Wang *et al.*, which does not describe that experimental data is introduced into a meta layer module that generates evaluation data which, in turn, influences processing at the optimizer, furthermore does not describe iteratively

processing experiment data from a plurality of experiments, using the meta layer module and the optimizer, until such time that an optimization goal is reached.

Withdrawal of the Section 102 rejections is, therefore, respectfully requested.

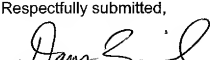
CONCLUSION

For the foregoing reasons, it is believed that all of the claims, as presently presented, are patentable.

The Examiner is invited to telephone the undersigned if it is believed that further amendment and/or discussion would help to advance the prosecution of the present application.

Reconsideration and allowance of claims 22-44 are, therefore, respectfully requested.

Respectfully submitted,



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